

10712258 09/20/05

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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

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NEWS 2 "Ask CAS" for self-help around the clock  
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NEWS 6 AUG 30 CASREACT - Enhanced with displayable reaction conditions  
NEWS 7 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY  
NEWS 8 SEP 22 MATHDI to be removed from STN

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:12:04 ON 01 OCT 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:12:52 ON 01 OCT 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 SEP 2005 HIGHEST RN 864353-93-5  
DICTIONARY FILE UPDATES: 30 SEP 2005 HIGHEST RN 864353-93-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

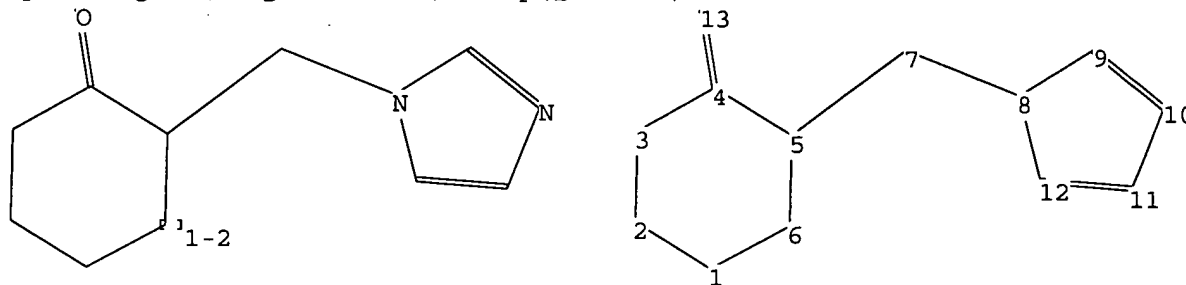
```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10712258.str



chain nodes :

7 13

ring nodes :

1 2 3 4 5 6 8 9 10 11 12

chain bonds :

4-13 5-7 7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-13 5-6 7-8 8-9 8-12 9-10 10-11

exact bonds :

5-7 11-12

isolated ring systems :

containing 8 :

Match level :

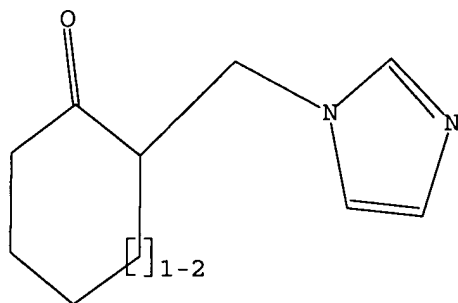
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:13:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 496 TO ITERATE

100.0% PROCESSED 496 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8584 TO 11256

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:13:17 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9119 TO ITERATE

100.0% PROCESSED 9119 ITERATIONS

24 ANSWERS

SEARCH TIME: 00.00.01

L3 24 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

161.33

161.54

FILE 'CAPLUS' ENTERED AT 15:13:25 ON 01 OCT 2005

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FILE COVERS 1907 - 1 Oct 2005 VOL 143 ISS 15  
FILE LAST UPDATED: 30 Sep 2005 (20050930/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 22 L3

=> s 14 and oxazolidine

3939 OXAZOLIDINE

1268 OXAZOLIDINES

4294 OXAZOLIDINE

(OXAZOLIDINE OR OXAZOLIDINES)

L5 2 L4 AND OXAZOLIDINE

=> d ibib abs hitstr tot

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STM

ACCESSION NUMBER: 2004:652673 CAPLUS

DOCUMENT NUMBER: 141:174173

TITLE: Process for the preparation of imidazolyl compounds

INVENTOR(S): Verbeek, Jan-Maarten; Van der Meij, Paulus F. C.

PATENT ASSIGNEE(S): Solvay Pharmaceuticals B.V., Neth.

SOURCE: U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXKCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004158077	A1	20040812	US 2003-712258	20031114
PRIORITY APPLN. INFO.:			EP 2002-79838	A 20021118
			NL 2002-1021939	A 20021118

OTHER SOURCE(S): MARPAT 141:174173

GI

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STM (Continued)

stirred for 2 h at 120° C to afford V.HCl in 77% yield. The method is esp. useful for the prepn. of selective neuronal 5-HT receptor antagonists, which are useful as anti-migraine and antipsychotic agents.

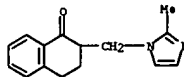
IT 697807-10-6P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

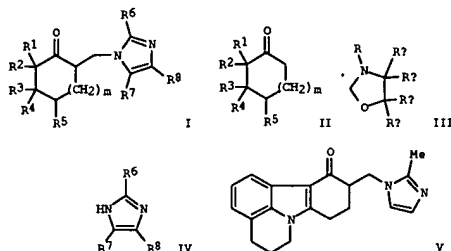
(preparation of imidazolyl compds.)

RN 697807-10-6 CAPLUS

CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(2-methyl-1H-imidazol-1-yl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl



AB The invention discloses a method for the preparation of imidazolyl compds., such as I [R1, R3 = alkyl, alkoxyalkyl, optionally substituted aryl or heteroaryl; R1R3 = fused homocyclic or heterocyclic system comprising one or more rings; R2, R4 = H, double bond (optionally part of an aromatic system); R5 = H, alkyl, alkoxy, alkoxyalkyl, halogen; R6, R7, R8 = H, alkyl; m = 1-2; R6 = H, alkyl, acid addition salts], by reacting a cyclic ketone of formula II with an oxazolidine derivative III (R = H, alkyl optionally substituted with OH or an optionally substituted aryl group; Ra, Rb, Rc, Rd = H, alkyl), followed by reaction with an imidazole IV. Thus, 5,6,9,10-tetrahydro-4H-pyrido[3,2,1-jk]carbazol-11(8H)-4-one and MeSO<sub>3</sub>H in BuOH were heated to 70° C and then treated with 3-oxazolidineethanol in BuOH, and the mixture was heated for 50 min at 80° C. Then, 2-methylimidazole in BuOH was added and the mixture was

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STM

ACCESSION NUMBER: 2004:453190 CAPLUS

DOCUMENT NUMBER: 141:23529

TITLE: Novel process for the preparation of imidazolyl compounds, particularly ondansetron, cilansetron, and analogs, using oxazolidine derivatives as formaldehyde equivalents in a Mannich-like reaction

INVENTOR(S): Verbeek, Jan-Maarten; Van Der Meij, Paulus F. C.

PATENT ASSIGNEE(S): Solvay Pharmaceuticals B.V., Neth.

SOURCE: PCT Int. Appl., 22 pp.

CODEN: PIXKX2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046116	A1	20040603	WO 2003-EP50841	20031117
W: AE, AG, AL, AM, AT, AU, AZ, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2504614	AA	20040603	CA 2003-2504614	20031117
EP 1565445	A1	20050824	EP 2003-811396	20031117
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			EP 2002-79838	A 20021118
			WO 2003-EP50841	W 20031117

OTHER SOURCE(S): CASREACT 141:23529; MARPAT 141:23529

GI

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STM (Continued)

as anti-migraine and antipsychotic agents, e.g., ondansetron and cilansetron. The method is superior to prior art Mannich processes using formaldehyde, which give tar-like byproducts when scaled up. For instance, 1,2,3,9-tetrahydro-9-methyl-4H-carbazol-4-one and MeSO<sub>3</sub>H in BuOH were heated to 90° and then treated with 3-oxazolidineethanol in BuOH, and the mixt. was heated for 50 min at 80°. Then, 2-methylimidazole in BuOH was added and the mixt. was stirred for 2 h at 120°. Extn. and crystn. gave V.HCl, i.e. ondansetron HCl, in 70.1% yield and ≥ 95% purity, with an addnl. 14.5% product in the mother liquor. Similar preps. of (±)-cilansetron HCl and another compd. are also given.

IT 697807-10-6P, 3,4-Dihydro-2-[(2-methyl-1H-imidazol-1-yl)methyl]-

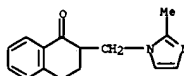
1(2H)-naphthalenone hydrochloride

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(target compound; improved preparation of imidazole 5-HT antagonists (ondansetron and cilansetron) using oxazolidine derivs. as formaldehyde equivalent in Mannich-like reaction)

RN 697807-10-6 CAPLUS

CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(2-methyl-1H-imidazol-1-yl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to an improved method for the preparation of

imidazolyl

compds. I [wherein: Ra, Rb = Cl-C6 alkyl, Cl-C6 alkoxyalkyl, optionally substituted aryl or heteroaryl; or RaRb = fused homocyclic or heterocyclic system comprising one or more rings; Ra'Rb' = H<sub>2</sub>, carbon-carbon double bond (optionally part of an aromatic system); Rc = H, Cl-C6 alkyl, Cl-C6 alkoxy, Cl-C6 alkoxyalkyl, or halogen; Rd = H or Cl-C4 alkyl; Re = H or Cl-C4 alkyl; m = 1 or 2; R1 = H or Cl-C4 alkyl; as well as acid addition salts]. The method is characterized in that a cyclic ketone of formula II reacts with an oxazolidine derivative III, followed by reaction with an imidazole IV, optionally followed by reaction with a suitable acid [wherein: R1, Rd, and Re = as given above; R = H, Cl-C4 alkyl optionally substituted with OH or an optionally substituted aryl group; R', R'', R''', and R'''' = H or Cl-C4 alkyl]. The method is especially useful for

the preparation of selective neuronal 5-HT receptor antagonists, which are useful

10712258 09/20/05

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

13.12

174.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

ENTRY

TOTAL

SESSION

CA SUBSCRIBER PRICE

-1.46

-1.46

STN INTERNATIONAL LOGOFF AT 15:15:23 ON 01 OCT 2005